

PROJECT NUMBER: 1754
PROJECT TITLE: Spectroscopic Studies of Tobacco and Smoke Components
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PERIOD COVERED: November, 1988

SOLUTION NMR

- A. Objective: Use NMR to determine the optical purity of nicotine.
 - B. Results: Experiments using β -cyclodextrin as a chiral shift reagent to produce chemical shift differences in racemic nicotine were not successful.
 - C. Plans: Additional experiments are planned where the nicotine will be protonated in order to facilitate the inclusion by the cyclodextrin. Another set of experiments using a derivative of tartaric acid as the chiral shift reagent will also be explored.
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- A. Objective: Use NMR to confirm the structure and purity of alkyl pyrazines used in flavor studies.
 - B. Results: ^1H and ^{13}C data were collected on an additional series of alkyl pyrazine derivatives. This series of compounds proved to have the correct structure and was of a high degree of purity (95+%). The trace amounts of water found in the previous series appears to be removed from this series.

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